Details of Research Proposal

(1) Area / Specializations of the Research:

Condensed Matter Physics (Nanomaterials)

(2) Topic: Study on Thermodynamic and Thermophysical Properties of Nanomaterials

(3)Introduction:

The nano materials are the bridge material between bulk and single molecular state. Due to smaller size, they have large surface area to volume ratio and hence they have more unsaturated atoms on their surface. Due to this unsaturation, nano materials have highly different physical and chemical properties from their bulk state[1].

Thermodynamic and thermophysical properties like cohesive energy, melting point, evaporation temperature,Debye temperature, melting entropy, specific heat, thermal conductivity etc, behave differently with reducing particle size [2-5]. The cohesive energy, melting temperature and Debye temperature show sharp reduction with decreasing size in nano range whereas specific heat shows the opposite behavior [6]. Hence, the study of these thermodynamic andthermophysical properties of nanomaterials is of much importance because it hasvarious applications in the fields of science and technology[7,8]. There are various models[9-13] to understand and explain these size dependent physical properties.The thermodynamic model developed by Qi and Wang in which they have assumed that the cohesive energy of nanomaterials is the sum of energies of interior and surface atom with the concept of dangling bond at thesurface has been used extensively [14].Thermodynamic and thrmophysical properties like cohesiveenergy, melting temperature, Debye temperature etc. have been discussed for different size with the help ofthis model.

(4) Proposed Problem:

The properties of solids are affected by the bonding between the constituent atoms and the bonding is characterized by the cohesive energy(CE). On the basis

of the cohesive energy, most of the physical properties of solids can be derived [15].There are various thermodynamic models which can be used to predict the cohesive energy. Some of the models can be mentioned as the Bond-Order-Length –Strength (BOLS) model[16],the Liquid Drop model[10],the Shi-Jiang model[17-19], Guishiers model [20] and Bond Energy(BE) model[9,12,21].

Most of the models developed by different groups of researchers to explain size and shape dependence of the thermodynamic and thermophysical properties are inadequate and unable to have its good agreement with experimental results. It seems that some important structural aspects affecting the thermodynamic and thermophysical properties have not been incorporated in above said models.

Our main objective is to modify the existing models by introducing suitable factors or properties to have the simulated results with good agreement with available experimental results.

(5)Methodology:

Inorder to simulate results with the available data for the various nanomaterials, we use mathematical computational software to find the values of the different properties taking the size and the shape as variable. With the help the software, we will use the graphical representation for size and the shape dependent behavior of the considered properties of the nanomaterials. We will also compare the simulated results with available experimental data. On the basis of our new models we will predict the expected thermodynamic and thermophysical properties of nanostructured materials which have not been calculated theoretically or investigated experimentally. For the simulation of results we will use following models and methods beside the use of MATLAB computations.

Many of the properties of the nanomaterials are claimed to be dependent on their cohesive energy. In this study we plan to use BEM with some modification for calculating the some of the physical properties of the nanomaterials.

(6) A brief review of the research work:

The special properties of nanomaterials ariseprimarily because of their surface to volume ratio. To account for the surfaceeffects rigorously, size, shape, and surface relaxation must beconsidered.As mentioned above, various models

have been proposed topredict the cohesive energy in order to study thethermodynamic and thermophysical properties of the nanomaterials.BOLS theory proposed by C.Q. Sun,et al is based on the assumption that the coordination number imperfection of an atom at a surface causes the remaining bonds of the lower coordinated atom to relax spontaneously; as such the bond energy rises. The bond energy rise contributes not only to the cohesive energy of the surface atom but also to the energy density in the relaxed region. BOLS premise has led to consistency between predictions and experimental observations of a number of properties of nanosolids[17].During the year 2002,the liquid dropmodel[10] was proposed on the assumption that the CE can be effectively represented byvolume and surface dependent terms;it hassuccessfully explained the size dependent melting temperature andstructuraltransition of nanoparticles[10,22].In 1994,Shi proposed a model,usingthe Lindemanncriterion,for the size dependentamplitude of the atomic vibrations of a nanosolid [17]and Jianggeneralized this model [19,20],predictions of which agree with some of the experimentalvalues[23].Based on the core−shell structure, Qi et aldeveloped a very simple model known as bond-energy model (BEM) for the CE of lowdimensionalsolids [9,12,22]. The model has enabled us to reproduce the size and shape dependence of a number of physical properties, such as meltingtemperature, melting entropy, melting enthalpy, ordering temperature, etc. [24].

(7)Schedule of activity:

Year wise plan is given below

First year

Ph.D. course-work has been completed in the first two semesters (four papers).

Second year

In the third semester,comprehensive examination along with the state of art has been taken.More than 100 literatures has been arranged and studied from different resources, research laboratories, library and internet etc.

In the fourth semester, the problem selection and the problem- specific review of literature is to be done. In this semester we shall try to solve problems related to

the thermodynamic and thermophysical properties of the nanomaterials with suitable model.

Third Year

In this year the work will be focused on the computation of thermodynamic and thermophysical properties of the nanomaterials and to validate the results with existing experimental data.It is also proposed to predict the cohesive energy, evaporation temperature, specific heat, thermal conductivity, melting entropy, melting enthalpy and thermo-elastic propertiesof nanostructured materials. After successful computation of these important properties we will communicate for publication in different reputed international journals.

Fourth Year

In the seventh semester, focus will be given to predict the magnetic properties, equation of state and Gruneisen parameter of nanostructured materials.After getting the work published, thesis writing and submission will be done for the award of Ph.D. Degree.

(8) References:

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Signature of the Candidate **Signature of the Supervisor**

Forwarded

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